2-Amino-5-methylbenzenesulfonic acid

88-44-8 | DTXSID7026526

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 148 °C

Global applicability domain: Inside

Local applicability domain index: 3.87e-01

Confidence level: 6.18e-01

Nearest Neighbors from the Training Set

Image not found

2-Amino-1-naphthalenesulfonic

acid

Measured: 180 Predicted: 187

Image not found

Salicylamide O-acetic acid

Measured: 221 Predicted: 207

Image not found

CHEMBL106848 Measured: 112 Predicted: 112

Image not found

4-[(3-

Hydroxypropyl)sulfanyl]benzene-

1-sulfonamide Measured: 117 Predicted: 111